Dynamic Model of Hydrogen in GaN

by **S. M. Myers and A. F. Wright**

Motivation—Hydrogen is incorporated into p-type GaN during MOCVD growth, producing highly stable passivation of the Mg acceptors. Complete acceptor activation by thermal H release requires temperatures that threaten material integrity, prompting compromises in device processing. At lower temperatures, forward bias of p-n junctions or electron-beam irradiation produces a metastable, reversible activation without H release. To understand and control such effects, we are developing a mathematical model of H behavior wherein state energies from density-functional theory are employed in diffusion-reaction equations. Previously, we used the greatly simplifying assumptions of local equilibrium among states and local charge neutrality to treat uniform materials at high temperatures. Now, an extended diffusion-reaction formalism includes nonequilibrium, and a simultaneous solution of Poisson's equation takes account of space charge, allowing H to be modeled in junction devices, under bias, and at room temperature.

Accomplishment—Calculations using density-functional theory identified the important lattice states of H as H^+, H^0, H^-, interstitial H_2, the neutral Mg-H complex, and, in n-type material containing Si donors, the neutral Si-H center. Formation energies were calculated for these states, together with local-mode vibrational frequencies affecting the H chemical potential and diffusion activation energies for the mobile species H^+, H^0, and H^-. Also, captured-electron energies were theoretically evaluated for H^+, H^0, and the Mg-H complex to elucidate the reaction path of the aforementioned metastable activation of acceptors in p-n junctions under minority-carrier injection. To describe the time evolution of the system, differential equations were developed for the time and depth dependent concentrations of the above H states as well as Mg^-, Si^+, conduction electrons, holes, and net charge. The resulting formalism is solved numerically. Among the properties of the solution is that it reproduces our earlier treatment of thermodynamic equilibrium, which was validated by measurements of H solubility, and also our prior modeling of thermal release, similarly found to be consistent with experiment.

Applications of our newly extended model are exemplified by results for the metastable activation of Mg acceptors in a p-n junction under forward bias. We find that interstitial H_2 is the only viable candidate for the state of the H produced in this treatment. Additionally, we have predicted the rate at which the metastable activation is reversed during heating, as shown in Fig. 1. These results indicate that half-hour isochronal anneals will begin to restore the passivation at about 350ºC, which agrees with published observations. As another example, the model shows H being strongly excluded from the space-charge region of a p-n junction, as seen in Fig. 2, leading to bias-driven H redistributions with device implications at temperatures extending below 100ºC.

Significance—Through modeling a range of observable behaviors in terms of states predicted by *ab-initio* theory, we are validating and refining the understanding of H in GaN. These calculations are more quantitative and comprehensive than past treatments of H in semiconductors. Results are clarifying trade-offs in device processing and have already influenced processing protocols.

Sponsor for work: BES, DP

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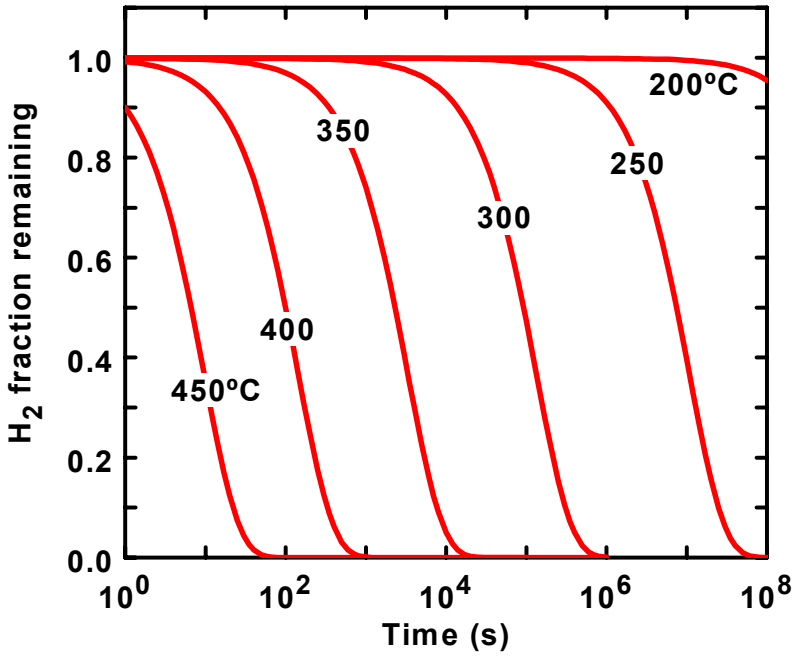

Figure 1. Theoretically predicted repassivation of Mg acceptors in GaN during annealing with no bias. Plotted versus time is the decreasing fraction of interstitial H_2 as the H returns to the acceptors and reforms the neutral Mg-H center.

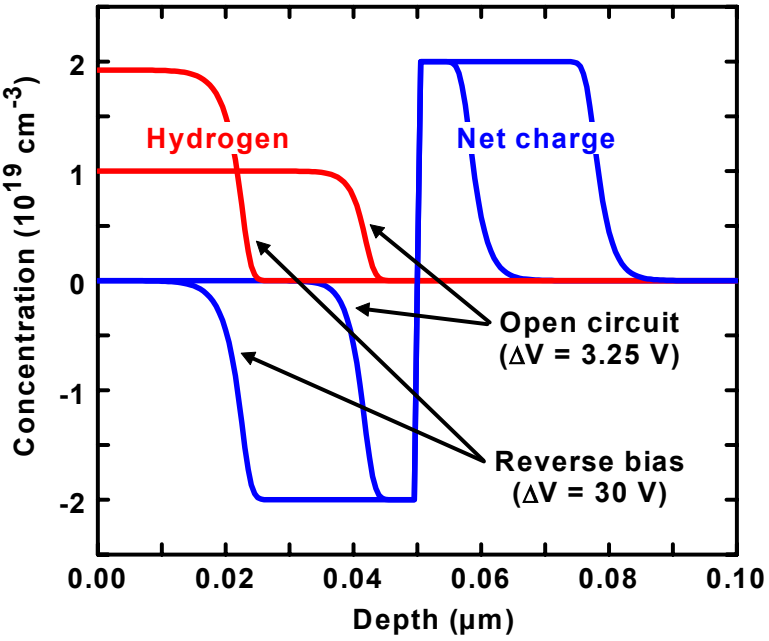

Figure 2. Theoretically predicted H redistribution in a p-n junction under bias with space charge also shown. In the model, H was first diffused into the p-type region from the surface under open circuit conditions and then caused to redistribute by the application of a reverse bias. The temperature is 400ºC, and the plotted depth profiles are for the asymptotically approached conditions.